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On Probabilistic Distribution of Forces in Granular Materials: A Statistical Mechanics Approach

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ABSTRACT

The contact force distribution in stressed grain piles under simple compaction or gravity has been studied intensively in recent years. In the present investigation, by performing discrete element simulations, it is found that the contact force distribution in a stressed granular packing can be described by a generalized form the Second Law of Thermodynamics involving minimization of a free energy functional containing an energy and an entropy component. The relative importance of energy and entropy is controlled by a parameter known as the “mechanical temperature”.

INTRODUCTION

The distribution of contact forces in random granular packings has been the subject of intensive investigations in the past decade [1-12]. Because of structural disorderness, the internal force distribution in random packings due to external loadings will not be uniform. In the rigid grain regime, it has generally been agreed that the large force distribution follows an exponential decay, while the small force distribution is more debatable [1-3]. In the compressible regime, the force distribution undergoes a gradual transition from the Maxwell-Boltzmann (strictly exponential) behaviour at small applied pressures to a Gaussian form at larger pressures [6].

This work is based on the belief that a satisfactory description of forces or indeed any other quantities in random granular packings should involve concepts from statistical mechanics [13]. In a stressed granular packing, there is a strain energy functional due to the applied loading but at the same time, there is also an entropy functional, due to the random nature of the system. We first postulate that mechanical equilibrium is reached when the energy contribution balances the entropy contribution. This condition is then used to derive the allowable forms of the contact force distribution in a stressed granular packing. The results are then compared with discrete element simulations.

GENERALISED CONCEPTS OF STATISTICAL MECHANICS

As Bagi [4] and Evesque [5] have pointed out, a force distribution $P(f)$ enables the definition of an entropy in the statistical sense

$$S = - \int_0^{\infty} P(f) \ln[P(f)] df. \quad (1)$$

Bagi and Evesque both argued that in a structurally random packing, the entropy in eqn. (1) should attain maximum value. This criterion always yields the exponential Maxwell-Boltzmann distribution which, in general, does not match the usually peaked experimental or simulated force distributions reported in the literature. If only entropy is maximized, the contribution of energy is ignored and this is against the spirit of the Second Law of Thermodynamics, one version of which states that when equilibrium is reached, the free energy defined by

$$F = E - \theta S \quad (2)$$

should reach a minimum, rather than the energy E alone should reach a minimum or the entropy S alone should reach a maximum. (θ here is a temperature scale.) In a stressed granular packing, the energy E should naturally be identified as the strain energy. A Hertzian contact force f between two contacting grains will be associated with a work done $W(f)$, and with a force distribution $P(f)$, this will be associated with an energy functional

$$E = \int_0^{\infty} P(f) W(f) df. \quad (3)$$

For a fixed temperature θ , the equilibrium force distribution should be obtained by minimizing F in eqn. (2), with E and S given by eqns. (3) and (1) respectively. This minimization should be subject to the following constraints for the probability distribution function $P(f)$:

$$\int_0^{\infty} f P(f) df = \bar{f} = \text{constant}, \text{ and } \int_0^{\infty} P(f) df = 1. \quad (4)$$

The minimization of F yields

$$P(f) = A \exp \left[-\frac{1}{\theta} (W(f) - \lambda f) \right], \quad (5)$$

where A and λ are normalization constants which make $P(f)$ satisfy (4).

The temperature scale θ in eqns. (2) or (5) is not the usual thermal temperature because the current mechanical problem is athermal. θ here simply controls the relative importance between energy and entropy, and is for convenience sake referred to as the “mechanical temperature”. $\theta = 0$ means that minimization of free energy F is equivalent to minimization of energy E , which will yield the perfect crystallinity behaviour. On the other hand, $\theta \rightarrow \infty$ corresponds to the Maxwell-Boltzmann or maximum entropy behaviour as stipulated by Bagi [4] and Evesque [5].

In a 2-D granular packing, where the grains are now parallel rods, the contact force between two grains is given by $f = \pi E_r a^2 / 2R$, where E_r is the reduced modulus, R the radius of the cylindrical grains, and a the radius of the contact zone [14]. The work done by f is

$W(f) = -\int_0^a f \cdot \frac{dr}{da} da$, where $r = 2\sqrt{R^2 - a^2}$ is the distance between the grain centers. $W(f)$ can be shown to be given by

$$W(f) = \frac{2\pi E_r}{3} \left[R^2 - \left(\frac{Rf}{\pi E_r} + R^2 \right) \sqrt{1 - \frac{2f}{\pi E_r R}} \right] \approx \frac{2f^2}{3\pi E_r}, \quad (6)$$

where the simplification at the end is accurate when f/E_r is small compared to unity. Substituting eqn. (6) into eqn. (5) yields a Gaussian form of the force distribution

$$P(f) = A \exp\left[-\kappa(\langle f \rangle - f_o)^2\right], \quad (7)$$

where $\langle f \rangle = f/\bar{f}$, \bar{f} being the mean force, $\kappa = \frac{2\bar{f}^2}{3\pi E_r} \cdot \frac{1}{\theta}$ is an inverse and dimensionless measure of the mechanical temperature, and A and f_o are normalization constants. Similarly, for a 3-D granular packing, the force distribution can be shown to be

$$P(f) = A \exp\left[-\kappa(\langle f \rangle^{5/3} - \lambda \langle f \rangle)\right], \quad (8)$$

where $\kappa = \frac{2}{5R} \left(\frac{3R}{8E_r} \right)^{2/3} \bar{f}^{5/3} \cdot \frac{1}{\theta}$, and A and λ are normalization constants. Figs. 1 and 2 show the equilibrium $P(f)$ as at different mechanical temperatures for 2-D and 3-D respectively.

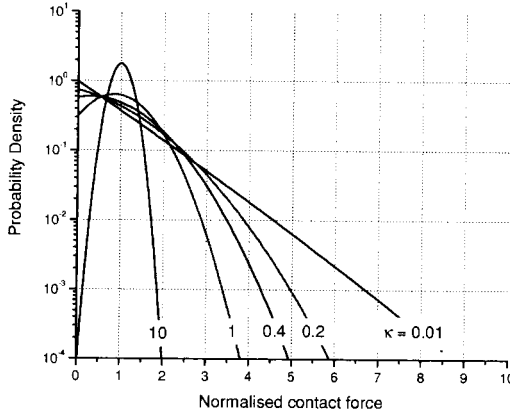


Figure 1. 2D equilibrium force distribution at different “mechanical” temperatures. κ is an inverse measure of the mechanical temperature θ (see text).

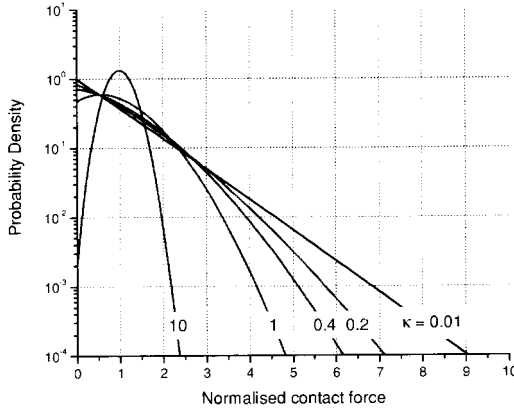


Figure 2. 3D equilibrium force distribution at different “mechanical” temperatures. κ is an inverse measure of the mechanical temperature θ (see text).

DISCRETE ELEMENT SIMULATIONS

Computer simulations were performed on elastic grains contained in a box, with compressive load applied from the top through a piston. Both 2-D and 3-D simulations were performed. The 2-D simulations were performed on 1×10^4 elastic grains, and the grain sizes distributed approximately uniformly throughout a range of $\pm 10\%$ of the mean value to prevent crystallization. For 3-D, 5×10^4 grains were simulated, and the grain size was uniform since it was observed that the structure did not crystallize easily. The Young’s modulus for 3-D was selected to be 200 GPa, and Poisson’s ratio 0.3. Only elastic Hertzian contact forces [14] were assumed, and friction was not included in the simulations.

Fig. 3 shows the simulated results for 2-D. It can be seen that the normalized force distribution is invariant with respect to the applied hydrostatic load over a four orders-of-magnitude change of load up to about 1 unit. Beyond 1 unit of load, the force distribution changed to another form with a smaller variance. Accompanying this change was an observed drastic change in the average number of contacts per grain, which remained roughly constant at the rigid-grain limit [15] of 4 when the load was smaller than about 1 unit, but increased to larger than 5 when the load was 10 units. The higher coordination at large loads corresponds to a more regular arrangement or increased degree of crystallinity of the packing. In fig. 3, the probability curves from 0.0001 to 1 unit of load can be fitted accurately by eqn. (7) with $\kappa = 0.2$. The curve at 10 units of load can be fitted accurately by $\kappa = 0.7$. The good fit in both cases indicates the validity of the theory above, namely, the equilibrium distribution corresponds to minimization of $F = E - \theta S$ at constant θ . The fitted results also indicate that κ is constant over a four orders-of-magnitude change in the applied load up to about 1 unit, but starts to decrease when the degree of crystallinity increases. From this observation, κ can be interpreted as a structure sensitive

parameter. Also, since κ is constant at constant structure, θ is proportional to \bar{f}^2 or to $(\text{load})^2$ at constant structure.

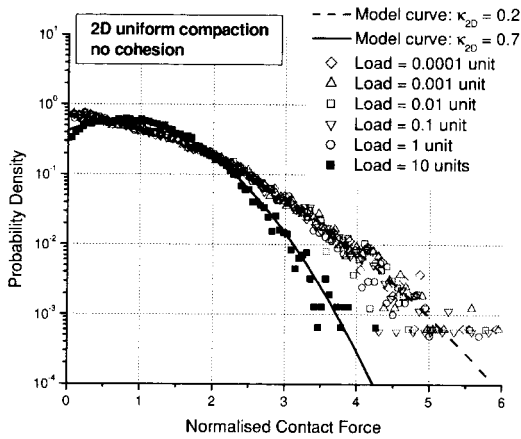


Figure 3. Computer simulation results of contact force distribution in 2-D under hydrostatic load. Contact forces are normalized by the mean value. 1 unit of load = $2 \times 10^{-3} E \bar{d}$, E = Young's modulus, \bar{d} = average grain size.

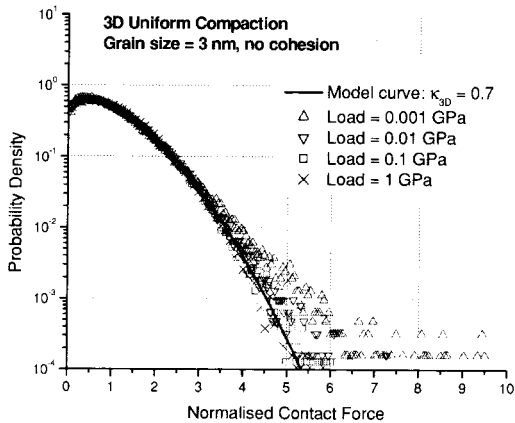


Figure 4. Computer simulation results of contact force distribution in 3-D under hydrostatic load.

The 3-D simulation results are shown in fig. 4. Here, it can be seen that the force distributions under applied pressure from 0.001 to 1 GPa are all invariant with respect to load, and can all be accurately fitted by eqn. (8) with the κ_{3D} parameter chosen to be 0.7.

CONCLUSIONS

In stressed granular packings, the internal force distribution due to external loading is not uniform. The internal force is associated with a strain energy functional and the distribution of forces enables the definition of an entropy functional. Computer simulation results of the force distribution show that equilibrium is governed by a compromise between the energy and entropy, i.e. the equilibrium force distribution is given by minimization of a free energy functional which is a mixture of energy and entropy. The mixity between energy and entropy is controlled by a parameter which is a mechanical analogue to temperature in a thermal system. The “mechanical temperature” is an increasing function of the applied stress.

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